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Process Systems Engineering developments in Europe from an industrial and academic perspective

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Keywords

Process systems engineering, industry, education, research, interface, perspectives

Highlights

- Process Systems Engineering insights from an industrial and academic perspective
- Challenges and opportunities for PSE improvements in academia and industry
- Critical factors affecting the progress of PSE and potential developments

Abstract

Process Systems Engineering (PSE) is a discipline that deals with decision-making, at all levels and scales, by understanding any complex process system using a holistic view and a systems thinking framework. A closely related discipline (considered usually a part of PSE) is the Computer Aided Process Engineering (CAPE) which is a complementary field that focuses on developing methods and providing solution through systematic computer aided techniques for problems related to the design, control and operation of chemical systems.

Nowadays, the 'PSE' term suffers from a branding issue to the point that PSE no longer gets the recognition that it deserves. In chemical engineering education the integrative systems frame for process design, control and operations is virtually absent. Its application potential in process industry lags relative to academic research progress and results. This work aims to provide an informative industrial and academic perspective on PSE (focused on the European region), arguing that the 'systems thinking' and 'systems problem solving' have to be given priority over just applications of computational problem solving methods. A multi-level view of the PSE field is provided within the academic and industrial context, and enhancements for PSE are suggested at their industrial and academic interfaces to create win-win situations.

1. Introduction

Process Systems Engineering (PSE) is a discipline concerned with methods and tools to support decision-making for the creation and operation of chemical supply chains, including the discovery, design, manufacturing, processing, and distribution of chemical products (Grossmann and Westerberg, 2000; Stephanopoulos and Reklaitis, 2011). In other words, PSE is all about rational decision-making, at all levels and length / time scales, by understanding complex systems using a holistic view and a systems thinking framework (Kiss et al., 2015). PSE is the wider field embracing Computer Aided Process Engineering (CAPE) as an important sub-domain where computing and information technologies play an essential role in finding solutions for problems of sustainable design, control and operation of chemical processes (Cameron and Lewin, 2009; Dimian et al., 2014, 2019; Kiss and Grievink, 2019). There are several excellent papers in literature, covering the PSE history, accomplishments, as well as developments of new methods and tools along the past decades (Grossmann and Westerberg, 2000; Klatt and Marquardt, 2009; Cameron and Lewin, 2009; Stephanopoulos and Reklaitis, 2011; Cameron et al., 2019; Grossmann and Harjunoski, 2019).

The issue of current standing of PSE in both academia and industry is a recurrent theme; see (Grossmann and Harjunoski, 2019). These authors offer a comprehensive review of the accomplishment of PSE over the past five decades, analyzing its impact both in academic research and industrial practice, including the existence of industrial consortia supporting major PSE research centers. Also the successful spin-out of new companies in the PSE core domain is mentioned. Yet, they point out that PSE suffers from lack of recognition in the broader setting of the natural and engineering sciences. A survey conducted by these authors among companies and universities has brought to light that its recognition in the process and automation industry is higher than in academia. The appreciation of PSE in industry is found to be very high. Obtaining enough academic research support to tackle the challenges ahead is voiced as an industrial main concern. A divergence in the current views on PSE between academia and industry is noted that can be countered by more interactions and coordination between them. The findings in this survey relate to the coverage of the polling, mainly universities (66 responses out of a total of 81) and companies (15 responses) in North and Latin America (75%) and to a lesser extent in Europe (18%).

This perspective paper – invited for the special issue of *Computers & Chemical Engineering* dedicated to the ESCAPE-29 conference – has several key contributions: it defines PSE and CAPE areas and their mutual relationship; it questions what makes PSE less effective in

chemical engineering (ChE) than it could potentially be; it shows that industrial as well as academic PSE have stronger & weaker points with known causes and amplified by deficient interactions with each other; it offers a model for enhanced PSE interactions between industry and academia covering key topics (e.g. sharing of industrial PSE problems with academia; knowledge generation by research & know-how transfer by moving PSE professionals between academia and industry; start-ups of companies with deep PSE expertise and tools for industrial services), and it concludes there is ample potential for improvement of effectiveness of PSE by working better across industrial and academic interfaces.

The analyses in this paper are primarily based on authors' experiences in a Dutch setting, but carry over well to other neighboring countries with similar industrial infrastructures. The Netherlands has a very large process industry (oil refining & fuels, chemicals, food) and many engineering consultancy and contracting offices. Its process industry is part of one of the strongest chemical clusters in the world, being among the top in EU – see Table 1. Four Dutch academic chemical engineering departments contribute to the knowledge infrastructure in this domain. Some of our findings are quite similar to those of Grossmann and Harjunkoski (2019) but also a few striking differences should be noticed.

2. Motivation

The international PSE research community has successfully established a vital science of engineering. Yet, its accomplishments are unevenly absorbed by the process industry and in educational programs. Application potential is lost and locally even branding issues arise. There is a known divergence between academia and industry due to different focus: research (funding and output) vs economic profit (Klatt and Marquardt, 2009). A key consequence is that industry considers most important the conventional core ChE disciplines, while academia (mainly driven by research funding / input) focuses on biotechnology, nanotechnology, or science-centered topics – as shown in Figure 1, left (Varma and Grossmann, 2014). Some barriers to more daring and effective use of PSE concepts, methods, models and tools (shown in Figure 1, right) include the following:

- The opportunities in making advancements in PSE seem to have moved from its interior (e.g. better models, faster computing) to external interfaces with other chemical engineering disciplines, such as process intensification (Tian et al., 2018), product innovation and engineering for multi-phase products (Harmsen et al., 2018).
- The huge application success of CAPE tools has shifted barriers in process engineering projects. In the past doing process data handling and engineering

computations fast and consistently was a key barrier. That kind of barrier has largely vanished, resulting in the emergence of other bottlenecks in: the organization of human work processes; the knowledge levels of process engineers being incommensurate with the capabilities of the tools; at the interface of technology and society with societal acceptance of technology applications.

This perceived discrepancy between the accomplishments of PSE research and its absorption by the chemical process industry and chemical engineering education will be further analyzed.

3. PSE in industry

Research, development & innovation enable the introduction of new or improved products and processes, and reduce the uncertainty about future performance to acceptable levels. PSE supports such reductions: business risks, time, cost & profit, environment, safety, health, social. Yet, PSE is typically perceived as a service provider to “customers” in company applications, making it difficult to put a value (not a cost) on its activities or quantify their contribution (Kiss and Grievink, 2019).

The industrial technology assessment models do take into account the probability of success when applying a new technology with a higher performance (or accounting for risk of failure), but it is rather unclear how does that tie in with PSE methods and tools for products and process innovations. Figure 2 shows a multi-level view of PSE positioning between the upper levels (determining the research directions) and the lower levels (tools and means to achieve the goals), with the “process” being seen as an optimized integrated production system, made up of one or more production plants (Kiss and Grievink, 2019). However, one clarification must be made with respect to the positioning of PSE vs process intensification (PI). Although these disciplines share a similar goal regarding the substantial improvement of chemical processes, there is quite a different set of science methods and skills used in PSE, which could be very useful to apply in process intensification (see Figure 3). Hence it is not surprising that many PSE groups worldwide have expanded their activity towards PI (Demirel et al., 2019).

Figure 4 shows that PSE has a key role in delivering more profit in shorter time, along all phases (e.g. research & development, engineering, process optimization, operation) taking into account all sustainability pillars (ten Kate, 2016). Of course, there is a trade-off between multiple criteria in Pareto type of optimization. Moreover, PSE reduces uncertainty along the way from idea to implementation, with the addition that there is also a reverse flow of information from an operational plant to the collection of process models. Plant data periodically collected in operational plants offer a rich base for “big data” analysis and

machine learning (Lee et al., 2018): e.g. finding patterns of behavior that can be exploited to improve process performances and be captured in updated models.

In PSE activities, the purpose shapes the models and these models have the role of transferable knowledge carriers (if the physical principles underlying the model are kept transparent in the structure of the equations). Setting up a model provides a structured approach to understanding the system. However, a combined approach of experiments supported by modelling is the most effective. PSE offers a structured approach in process and product development: guiding the lab-scale experiments, interpreting the experimental observations, and translating the results into the desired outcome.

A common problem in making a value assessment of contributions of PSE to technological advancements of products and processes is their intertwining with other contributions (e.g. by equipment engineering advances) to the overall project goal. Grossmann and Harjunkoski (2019) point out that: *“It is crucial to analyze the entire value chain, understand the relationships between different sub-systems and focus on the overall improvement.”*

Given the substantial contributions by PSE to technological advancements one may ask: how is PSE perceived among chemical and process engineering professionals? It appears that many industrial professionals have no idea about PSE, but they do know about process design, modelling, simulation, optimization, control, etc. These topics have been taught at the university in separate courses without the interactions in an integrative frame. It is quite likely also related to the way in which the process design and engineering activities are compartmentalized in the engineering divisions of companies. This observation is corroborated by the response to a question in a recent survey of the use of PSE skills in the Dutch process industry. This survey was conducted among PSE professionals and managers in the Dutch process industry (Grievink and Van der Ham, 2019). The question was about recognition of PSE as a professional field of activity in process technology & engineering within companies. Out of the 24 responses to this question 55% said PSE is an unknown term in their company, while they do perform process design / control / optimization studies, segregated by departmental boundaries. Another 16% indicated another name than PSE was in use within their company for the same professional field, while the remaining 29% indicated PSE is indeed known as the name of a core activity in their company.

This survey also revealed a clear appreciation for the model- & computing based (CAPE) activities in companies, while the conceptual power of a systems approach (main feature of PSE) was underrated or underutilized. The word ‘systems’ seems to be suffering from its generality and therefore from loss of meaning in a particular context. This issue is also

recognized with the German “*Systemverfahrenstechnik*”. Kuhn and Briesen (2019) articulate this apparent loss of meaning and tackle it by means of a philosophical reflection and by assigning some clear attributes (function, structure, components, hierarchy, surroundings) to systems. It aims at giving distinctive power to Process Systems Engineering in relation to the other chemical engineering disciplines.

Regardless the modest current visibility of PSE in the Dutch process industry there is confidence in its future contributions. Some future challenges reported in the Dutch survey involve (ranging from short to longer term): deeper automation of handling of process engineering data flows over the successive work stages in a distributed multi-location working environment; encapsulation of new Process Intensification techniques in PSE tools; integration of product & process development & designs, electrification of processes, sustainable production cycles with decarbonization. The main threat that companies express in the Dutch survey is loss of their PSE experts as well as losing strength in competition to rivals with a stronger PSE knowledge base. This is acute because industrial PSE experts are rather scarce in the Dutch chemical engineering community. Maintaining a good PSE skill base is of vital importance to companies especially in the context of current challenges related to e.g. artificial intelligence, augmented reality, industry 4.0 and 5.0, big data, etc.

4. PSE in academia

Figure 5 illustrates the career span and life-long learning for PSE professionals at the interface of industry and academia, with a required exchange of professionals between academia & industry (Kiss and Grievink, 2019). But in the academic world, one must make a distinction between the academic research agenda for PSE, and the teaching / education in PSE topics.

4.1 PSE academic research

PSE research includes: spanning a wider ranges of physical scales in processes & supply chains; broader range of feedstocks; integration of process intensification and PSE; circular systems: integration in design & operation of product manufacturing, product application, recovery and recycling, medical process systems; multi-scale modelling and computing; uncertainty in design & engineering. Major achievements of PSE include the development of methodologies and tools to support process modelling, simulation and optimization (MSO). But MSO technologies have become a commodity; they are not a distinguishing research feature of the PSE field any more (Klatt and Marquardt, 2009). Hence PSE has to play a supportive role to the other engineering sub-disciplines (such as product engineering and

process intensification) that focus on smaller scales with specific objects. Examples of such objects are multi-phase products and formulations, multifunctional internals for process equipment, micro-scale devices for power generation, etc. The proper integration of such objects in products and/or processes is certainly part of PSE area. Also, a large-scale energy transition with electrified processes and inherent dynamic operations offers challenges.

The transfer of research results from academia to industry goes in two ways: by the human mind (of PhD and PDEng students) and by scientific papers and presentations. In practice, the recruiting of PhD students by companies is the more effective way of knowledge transfer, getting the means with the master mind. The practical quality of the academic research also depends on the quality of the research problems being worked on. It is a dual way. When industry could commit itself more to assistance in framing research problems from the application and knowledge transfer perspectives it is quite likely that academic researchers can afford to pay more attention to these aspects.

4.2 PSE education

PSE education is part of the broader chemical engineering education. There are several pressing reasons to rethink and revise the traditional chemical engineering curriculum tailored to large scale manufacturing processes for “simple” products. The products are “simple” in the sense of consisting of a homogeneous mixture of well-defined chemical components in a single thermodynamic phase. The following (non-exhaustive) drivers for change exist:

- Strong advances in the basic sciences (chemistry, physics, biology) leading to
- Understanding and control of physical / chemical events at micro- and nano-scales.
- Broadening of the product spectrum, including structured inhomogeneous products.
- Unparalleled advances in modelling, computing & data processing capabilities.
- Widening of the process concept from process plants to include smaller scale devices.
- Forced dynamics acting on production processes as part of interacting supply chains.
- Emerging energy transition and decarbonization.
- Non-uniform resource distribution and uneven resource demands
- Socio-Techno-Economic-Political nexus

In their search for structure in PSE education (Cameron et. al., 2019) start by referring to the Grand Challenges for Engineering and stressing the importance of systems approaches because of the inherent complexity and interdisciplinary nature of these challenges. This call for systems approaches is also prominent in a MIT coordinated effort on Frontiers in

Chemical Engineering Education (abbr. FiCHEE) as to renew the chemical engineering undergraduate curriculum (Armstrong, 2006). Three leading principles to organize this curriculum are mentioned: 1) molecular transformations; 2) multi-scale analysis and 3) a systems approach. The latter is needed to deal with dynamics, complexity, uncertainty, and external factors at all relevant scales. In the corresponding proposal for the main structure of a new curriculum (see figure 5 in Varma & Grossmann, 2014) the systems component is present from the first year onwards. It is offered in layers of increasing sophistication. This approach reflects and honors past experiences in PSE education that one has to gradually build up the complexity, while the systems engineering aspects can be introduced from first year in BSc / BEng onwards.

Concerning core elements of PSE education, Cameron et. al., (2019) recommend: system modeling and simulation; optimization; dynamics and control; and process and plant design. They also stress that *“the envisaged curriculum should provide an embedding of the knowledge into a general framework that can be applied to new problems and domains”*. When teaching the PSE core elements in succession (e.g. process analysis, product & process synthesis and design, dynamics and control, optimization of process operations within supply chains, safety and reliability engineering) one could also emphasize the interdependencies between decisions made in these (PSE) activities.

Having emphasized the importance of the system concept as the general framework that embraces above four core activities a strong foundation is laid for PSE education to effectively deal with ongoing and new expansions in chemical engineering. One can think of product engineering (e.g. of functional catalytic structures at nano/micro-scales), process intensification, energy systems engineering, interconnected processing functions of body organs, bio-based and circular economy (Avraamidou et al., 2020). Such an approach will benefit the students, the industrial companies hiring the graduates, and also foster the systemic innovations in (bio)chemical production systems for our societies at large.

A special word on education is in order for a typical feature of the Dutch academic engineering system, offering more leeway to advanced levels of engineering skills and applications. The left hand side of Figure 5 mentions three programs after BSc, being MSc (2 years) and then a choice between PhD (+4 years) and PDEng (+2 years). While a PhD is research oriented with a focus on shifting the frontiers of knowledge, the Professional Doctorate in Engineering (PDEng) program has a different focus. It aims at shifting the frontiers of applications of technology and engineering design. This two-year program has one full year devoted to broadening and deepening the theoretical base, while the second year

is filled with two major design projects, the latter always in collaboration with an industrial party who typically hosts the PDEng student.

The PDEng programs exist since 1990 and have become highly appreciated by the Dutch industry. There are four PDEng programs running in the chemical engineering and the biotechnology domain. They give room to some advanced elective PSE related courses. Examples are: heat & mass integration, design of plant-wide control structures, optimization in chemical engineering, mastering comprehensive structural approaches to conceptual product and process designs by means of the Delft Design Map (Harmsen et al., 2018).

While the structures and content for PSE education look fine there is currently often a painful “expertise pinch” in chemical engineering programs with respect to the teaching of PSE topics and the research in the department. It corresponds to a situation mentioned by Varma & Grossmann (2014) that in some USA chemical engineering departments “*the teaching of process design has been largely outsourced to adjunct faculty (typically, retired engineers from industry)*”. Due to substantial shifts in research funding from the sciences of engineering towards the natural sciences over the last decade, faculty with PSE expertise has become rare in The Netherlands. External (international) and industrial experts in PSE had to be hired to teach certain courses. However, the outlook for the future seems brightening.

There is increasing awareness within chemical engineering programs of the complexities and the system aspects in relation to the Grand Challenges by the four categories sustainability, health, security, and joy-of-living. Out of these, sustainability is the key one for the process industries and this implies that PSE should be more actively applied in industrial practice (Bakshi, 2019). This is contingent upon the following four ingredients that we consider essential for a successful education of chemical engineers with good PSE skills:

- A systems frame to embed and connect the four main activities in PSE involving modelling, design, dynamics& control and optimization of operations.
- Competent PSE faculty for teaching and who are conversant with industrial applications.
- Transfer of PSE skills through training in post-graduate educational programs (third cycle in the European Bologna education model). The Dutch PDEng programs offer a successful example with active participation by industrial parties.
- Research activities in PSE domain to develop & train next generation PSE experts.

Our overall view is that the contribution of PSE in the chemical engineering education is entering a new era of growth by thorough reflections on its content and new urgency due to

societal needs. The range of contents of PSE will further expand at the extreme ends of the size & time scales. How to deal with systems engineering aspects of processes at tiny (nano/micro) scales, driven by the rapid advances in the natural sciences? Also more attention is called for systems engineering of large-scale manufacturing complexes. This is needed for a long-term sustainable performance in the face of many uncertainties, risks and with often conflicting performance objectives. The new urgency is in re-designing the process industry to achieve carbon-neutral production at increasingly larger scales to satisfy the material needs of a growing world population. This is a very grand role for PSE indeed and it will certainly be fostered by closer research interactions between industry and academia and even public policy agencies.

5. PSE perspectives

Enhanced PSE interactions between industry and academia needs to cover: sharing with academia of abstracted generic industrial PSE problems (education and research); knowledge generation by academic research with selective transfer to supportive industrial partners (see framework in Figure 6); as well as knowledge and know-how transfer by moving PSE professionals between academia and industry; and start-ups of small companies (providers) with deep PSE expertise and tools for industrial services (Kiss and Grievink, 2019). Note that offering more advanced PSE tools (pushed by academia usually) is rarely effective for the industrial practice without additional precautions and preparations. Hence a key question remains: how to deal with PSE projects involving academics and industrialists? What needs to change for more enhanced interactions of both worlds includes:

- *Industry*: awareness from companies that the external development power is actually many times greater than internally in a company (although internally more focus on specific goals can be attained). Open innovation projects can accelerate the technology transfer of novel developments from the academic world into the industry.
- *Academia* needs to accept that the generation and use of engineering knowledge goes wider than writing good publications on theoretical and computational advances. Critical aspects of knowledge transfer and implementation need to be taken into account in the research approaches. The ultimate rationale for generating engineering knowledge is its application by joint projects and collaborations with industry.

An important aspect here is that industrially funded research is critical, especially in times of reduced public funding when new funding models that are better fit-for-purpose must be identified. Otherwise there is a risk that the academic research is not in the core of the

industrial developments. A successful example of such funding models is the Dutch Institute for Sustainable Process Technology (ISPT). This institute operates clusters of joint projects (in various specific areas, e.g. PSE, Industry 4.0, Industrial Fluids Processing, Utilities and Optimal Use of Heat) involving several companies that contribute financially to joint projects which are partly subsidized by public funding from Top Knowledge Institutes (TKI).

A good collaboration between academia and industry is essential for sustained success, but acceptance and good practical use of advanced PSE tools requires knowledgeable engineers and managers, so the role of the human factor is critical. Clearly, there is a need for well-trained PSE graduates from academia for successful identification, implementation and maintenance of PSE applications in companies. In this respect, some modifications to the university curriculum would be required to emphasize PSE studies, as backbone of chemical engineering. This could be in the form of specific PSE courses (which are not fully available at any university) in the first and last year, or at least in the form of PSE introductory lectures in the first year, followed by several reinforcements of PSE along other courses (e.g. Process Design, Process Control, Process Optimization, Design Project) and some overview lectures on PSE at the end of the studies. In addition, these graduates can be trained as part of a joint development and application process.

In the review of this article the challenging question was posed: *“if PSE is already applied so broadly that a natural host is missing and should it become a completely individual discipline by itself?”* One can consider PSE from the higher level of general Systems Engineering (Haberfellner et al., 2019). This is an interdisciplinary field that focuses on how to design and manage complex systems over their life cycles, and it uses systems thinking principles to organize this body of knowledge. An engineered system is the outcome of such efforts, and it can be defined as a combination of components that work in synergy to collectively perform a useful function. The generic attributes of a system cover the following: goals, resources to be transformed, functions, components, connections, network structure, hierarchy, boundaries, surroundings, as well as scenarios under which a system must be able to perform its functions. In the particular case of PSE, the word *“Process”* refers to an interactive sequence of transformations of multiple physical / chemical resources (e.g. energy, molecules) under guidance of information processing elements that transform measured data into useful information for human supervision to meet societal useful manufacturing goals. Of course, expanding on the definition of resources and transformations, one could cover e.g. data processing in software engineering as another form of systems engineering, or when using exclusively electricity as a resource to arrive at power systems. However, in our view the P (*Process*) in PSE links it

strongly to chemical engineering and its focus on chemical and physical transformations of materials and associated energy conversion effects. It is hard to think of a generalization by which PSE would become an independent discipline beyond chemical engineering and still be different from the general Systems Engineering discipline, or say, Operations Research. The actual development dynamics sits in the widening scope of chemical engineering and hence in the scope of PSE. As mentioned earlier in this article, the domain of chemical engineering is expanding to cover new types of processes beyond the (bio-) chemical / biotechnological manufacturing sectors, such as processes in biological living systems. Another lateral extension is possible at the interface between chemical engineering and other engineering disciplines. This could likely involve processes utilizing functional components from various engineering domains. In that case PSE would become a strong contributor to generalized “*Manufacturing Systems Engineering*”.

6. Conclusions

PSE contributed significantly to chemical engineering, by providing MSO technology to address demanding and large-scale process problems in academia and industrial practice. Systems thinking and problem solving are indispensable in the academic education of chemical engineers and also in the industrial practice. Industry mainly focuses on profitability and sustainability, while academia aims at scientific progress, causing a potential gap between industrial practice and academic research. Sustainable success of PSE requires consistent co-operations between academia and industry, certainly in view of the grand challenges of the next decades. PSE is a key enabler for process and product innovation, and has a bright future with sustainable impact on the chemical engineering sciences and on industrial manufacturing processes. PSE must consider new opportunities in other areas, while maintaining its identity (e.g. model-based systems thinking) in an ever-changing context. Educating enough skillful process systems engineers remains a critical factor to the impact of PSE as a research and application area supporting successful industrial innovations.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Tables

Table 1. Chemical industry overview in top EU countries (Data source: Landscape of the European Chemical Industry, CEFIC, 2018)

Country	Companies	Employees	Capital spending	R&D investment	Turnover
Germany	2,000	447,064	7.4×10^9 €	10.5×10^9 €	184.7×10^9 €
France	3,335	165,000	n/a	n/a	70.0×10^9 €
Belgium	720+	90,000	2.1×10^9 €	4.0×10^9 €	65.0×10^9 €
Spain	3,000	193,500	2.1×10^9 €	n/a	63.1×10^9 €
U.K.	3,460	140,000	4.7×10^9 €	6.3×10^9 €	59.5×10^9 €
Netherlands	470	57,000	n/a	0.75×10^9 €	55.0×10^9 €
Italy	2,800	108,100	1.6×10^9 €	0.52×10^9 €	52.0×10^9 €

Figure captions

Figure 1. Industrial importance of PSE topics (left). Methods and tools for PSE (right).

Figure 2. Multi-level view of PSE positioning

Figure 3. Process intensification (PI) vs PSE science methods and skills area

Figure 4. Role of PSE along all phases of plant development and exploitation

Figure 5. Career span for PSE professionals in academia and industry

Figure 6. Industrial vs academic PSE projects

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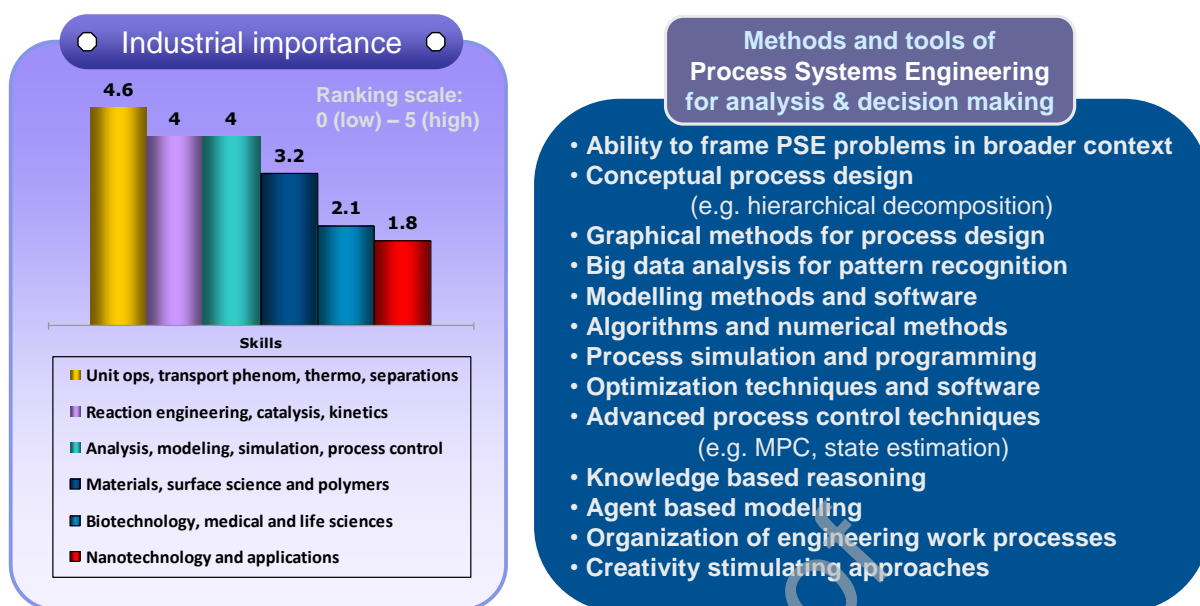


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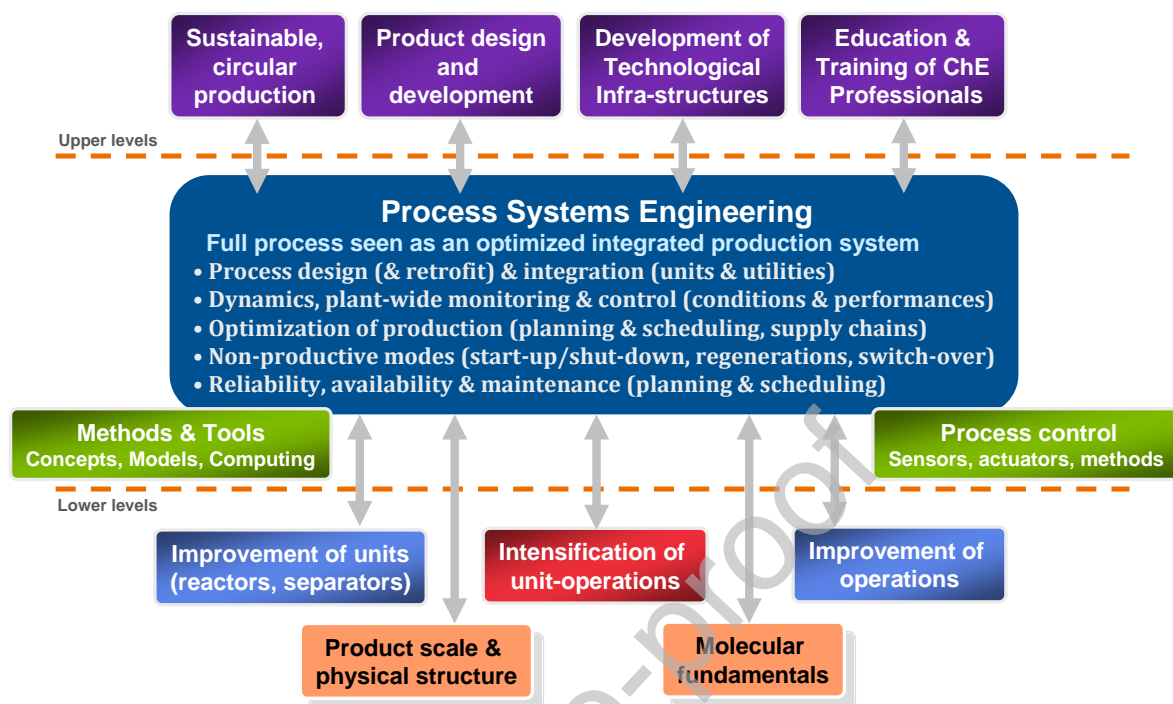


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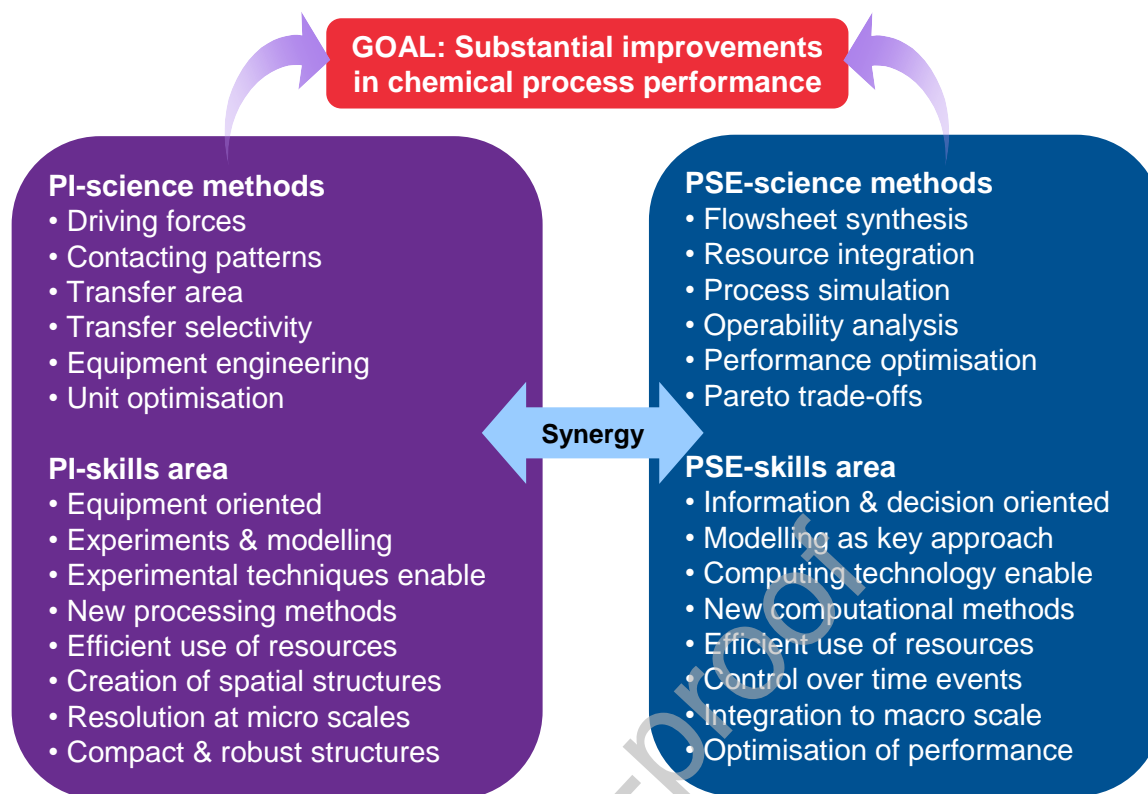


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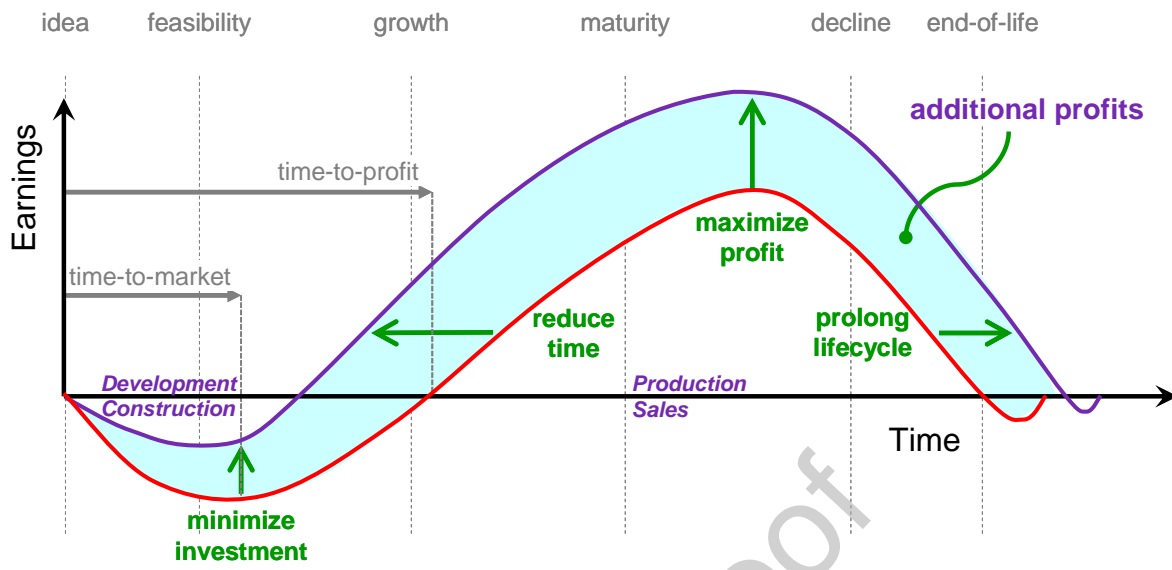


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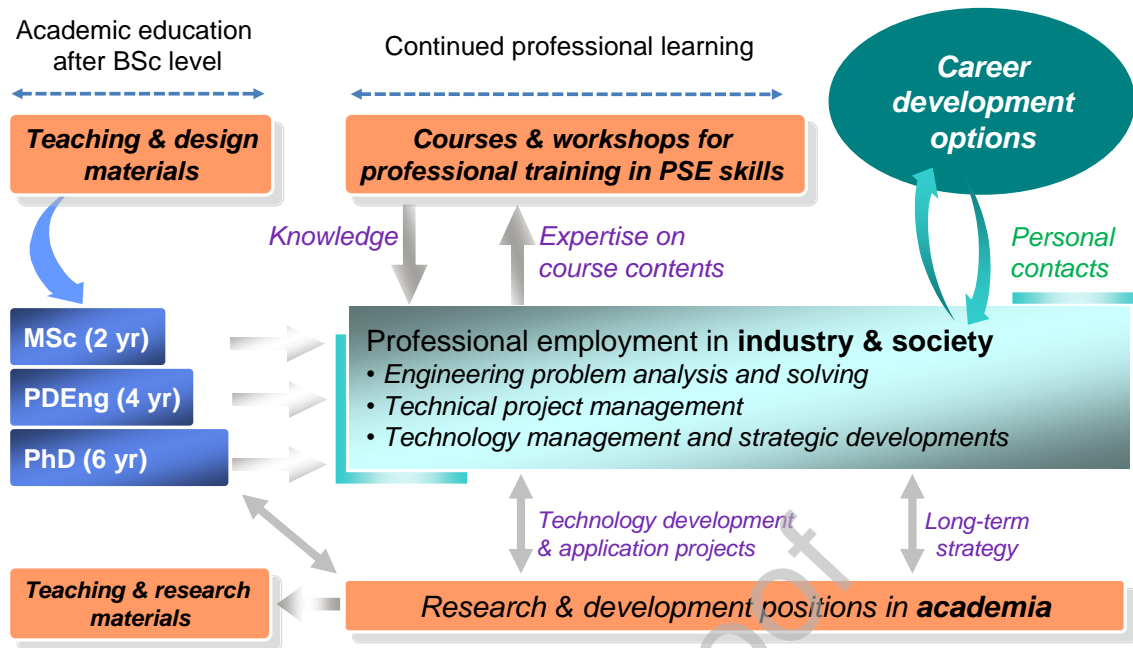


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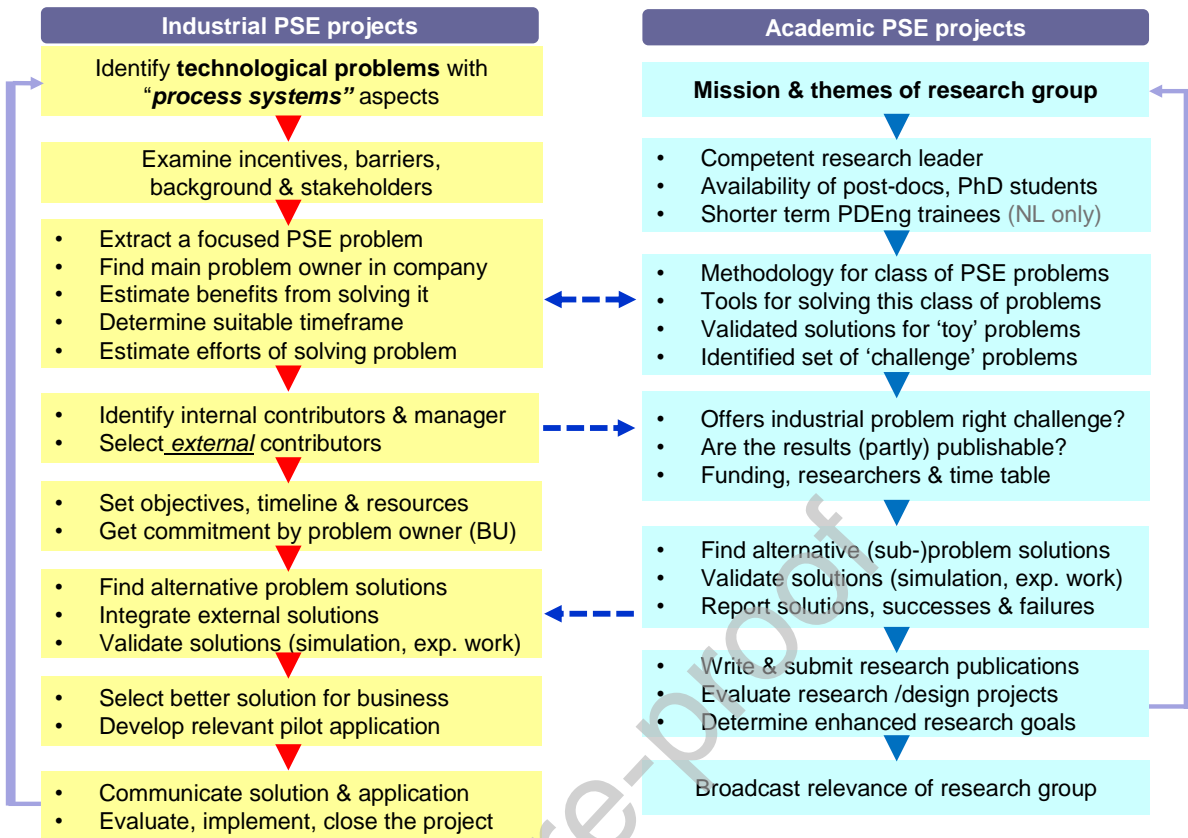


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